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=> fil hcaplus
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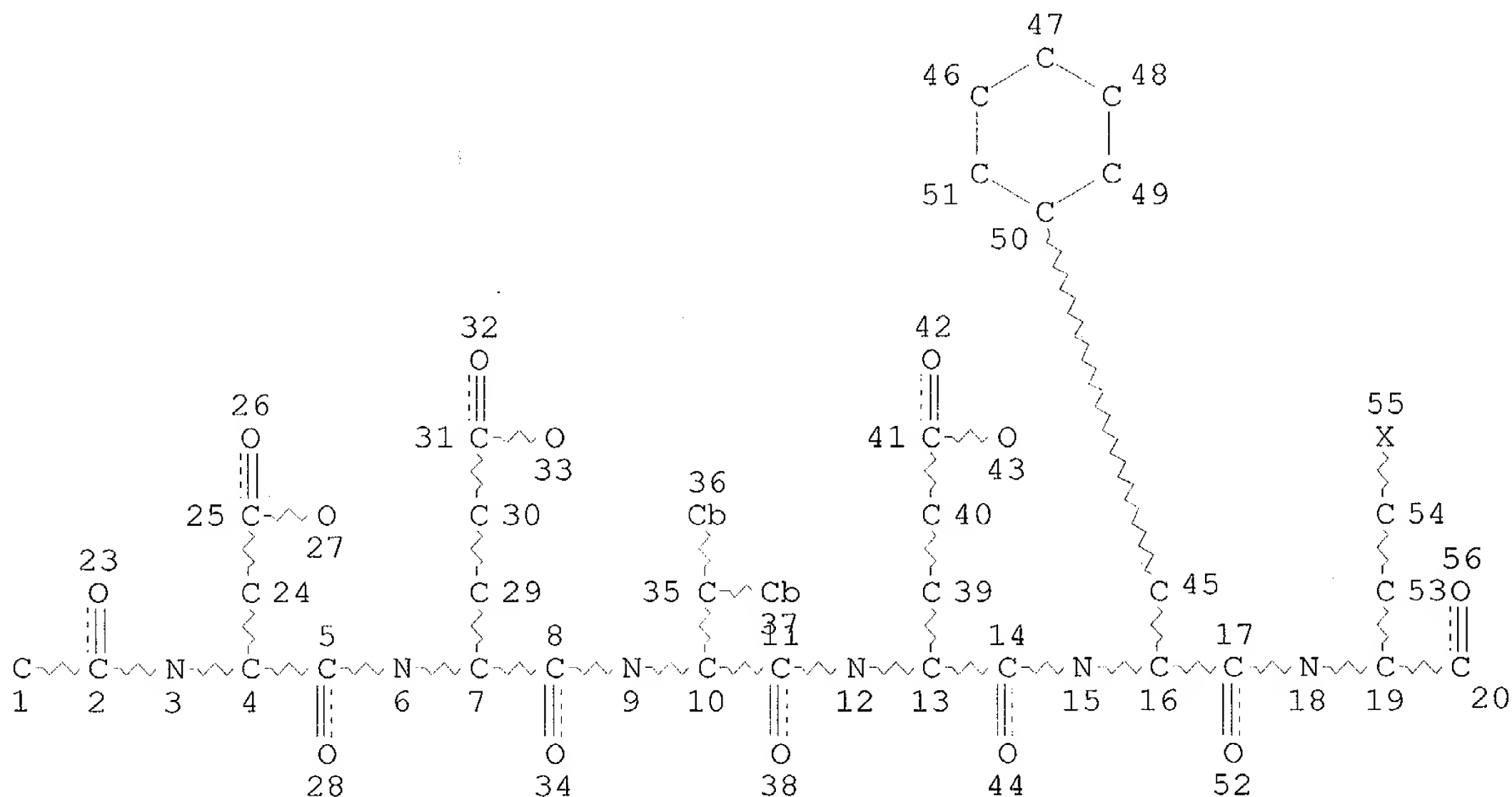
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FILE COVERS 1907 - 29 Sep 2003 VOL 139 ISS 14
FILE LAST UPDATED: 28 Sep 2003 (20030928/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3 STR
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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 54

STEREO ATTRIBUTES: NONE

L5 23 SEA FILE=REGISTRY SSS FUL L3
L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L5

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=> d ibib abs hitrn l6 1-6

L6 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:777963 HCAPLUS
DOCUMENT NUMBER: 137:295254
TITLE: Preparation of peptide inhibitors of hepatitis C virus
NS3 protease
INVENTOR(S): Colarusso, Stefania; Gardelli, Cristina; Gerlach,
Benjamin; Harper, Steven; Koch, Uwe; Matassa, Victor
Giulio; Muraglia, Ester; Narjes, Frank; Ontoria,
Ontoria Jesus Maria; Petrocchi, Alessia; Ponzi,
Simona; Stansfield, Ian; Summa, Vincenzo
PATENT ASSIGNEE(S): Istituto di Ricerche di Biologia Molecolare P.
Angeletti Spa, Italy; et al.
SOURCE: PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002079234	A1	20021010	WO 2002-EP3435	20020326
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				
PRIORITY APPLN. INFO.:			GB 2001-7924	A 20010329
OTHER SOURCE(S):			MARPAT 137:295254	
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I, II, and III [X = CH₂, O; Y = CRa₂, where Ra = H, OH, CO₂H, alkyl, (hetero)aryl, (hetero)aralkyl, or CRa₂ = cycloalkyl; Z = (un)substituted (hetero)aryl; R₂ = alkyl, fluoroalkyl, or CH₂SH; R₃ = (un)substituted alkyl, (hetero)aryl, (hetero)aralkyl, or together with NRc forms a ring; R_c = H or alkyl or NRc together with R₃ forms a ring; R₄ = alkyl, alkenyl, (hetero)aralkyl, (hetero)aryl or an acidic group; R₅ = (un)substituted carbamoyl, acyl, carboxylic ester, oxalyl, or sulfonyl group, which may be attached to an amino acid or a di- or tripeptide; R₁₃ is a group contg. .ltoreq. 25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms and .ltoreq. 9 other heteroatoms which may be the same or different; R₁₇ is H, alkyl, alkenyl, (hetero)aryl, (hetero)aralkyl, OH, alkoxy, aryloxy, (hetero)aralkoxy, thioether, sulfonyl or sulfoxide group; R₁₈ is a group contg. .ltoreq. 25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms and .ltoreq.

9 other heteroatoms which may be the same or different] and their pharmaceutically-acceptable salts or esters were prepd. as inhibitors of the hepatitis C virus (HCV) NS3 protease. Thus, i-BuO₂C-Glu-Leu-Cys-NHCH₂CH₂C₆H₃Cl₂-2,4 was prepd. by the solid-phase method and showed IC₅₀ 10 μ M for inhibition of NS3 protease.

IT 467440-27-3P 467440-28-4P 467440-45-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:116982 HCAPLUS

DOCUMENT NUMBER: 137:47425

TITLE: Evolution, synthesis and SAR of tripeptide .alpha.-ketoacid inhibitors of the hepatitis C virus NS3/NS4A serine protease

AUTHOR(S): Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Muraglia, Ester; Conte, Immacolata; Stansfield, Ian; Matassa, Victor G.; Narjes, Frank

CORPORATE SOURCE: Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 705-708

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:47425

AB N-Terminal truncation of the hexapeptide ketoacid MeCO-Asp-Glu-NHCH(CHPh₂)CO-Glu-NHCH(CH₂c-C₆H₁₁)CONHCH(CH₂CHF₂)CO₂H (all-L stereochem.) (c-C₆H₁₁= cyclohexyl) gave rise to potent tripeptide inhibitors of the hepatitis C virus NS3 protease/NS4A cofactor complex. Optimization of these tripeptides led to ketoacid BOC-NHCH(c-C₅H₉)CO-Leu-NHCH(CH₂CHF₂)COCO₂H (all-L stereochem.) (BOC = tert-butoxycarbonyl, c-C₅H₉ = cyclopentyl) with an IC₅₀ of 0.38 μ M. The SAR of these tripeptides is discussed in the light of the recently published crystal structures of a ternary tripeptide/NS3/NS4A complexes.

IT 262437-54-7

RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

(prepn. and structure-activity relationship of tripeptide ketoacid inhibitors of hepatitis C virus serine protease)

IT 262437-54-7DP, derivs.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and structure-activity relationship of tripeptide ketoacid inhibitors of hepatitis C virus serine protease)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:116981 HCAPLUS

DOCUMENT NUMBER: 137:149812

TITLE: A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease

AUTHOR(S): Narjes, Frank; Koehler, Konrad F.; Köch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.

CORPORATE SOURCE: Department of Chemistry, MRL Rome, IRBM, Rome,

SOURCE: Pomezia, 00040, Italy
Bioorganic & Medicinal Chemistry Letters (2002),
12(4), 701-704
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The difluoromethyl group was designed by computational chem. methods as a mimetic of the canonical P1 cysteine thiol for inhibitors of the hepatitis C virus NS3 protease. This modification led to the development of competitive, non-covalent inhibitor AcAspGlu-NHCH(CHPH2)CO-Glu-NHCH(CH2C6H11)CONHCH(CH2CHF2)R (I, R = CHO) Ki 30 nM and reversible covalent inhibitors (I, R = CO2H) Ki 0.5 nM; and (I, R = COCO2H) Ki* 10 pM.

IT 252355-84-3 252355-85-4 252355-86-5
262437-54-7 444990-66-3 444990-67-4
444990-68-5 444990-69-6 444990-70-9
RL: PAC (Pharmacological activity); BIOL (Biological study)
(designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:352482 HCAPLUS

DOCUMENT NUMBER: 133:189820

TITLE: Probing the active site of the hepatitis C virus serine protease by fluorescence resonance energy transfer

AUTHOR(S): Fattori, Daniela; Urbani, Andrea; Brunetti, Mirko; Ingenito, Raffaele; Pessi, Antonello; Prendergast, Kristine; Narjes, Frank; Matassa, Victor G.; De Francesco, Raffaele; Steinkuhler, Christian

CORPORATE SOURCE: Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Rome, 00040, Italy

SOURCE: Journal of Biological Chemistry (2000), 275(20), 15106-15113
CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A serine protease domain contained within the viral NS3 protein is a key player in the maturational processing of the hepatitis C virus polyprotein and a prime target for the development of antiviral drugs. In the present work, we describe a dansylated hexapeptide inhibitor of this enzyme. Active site occupancy by this compd. could be monitored following fluorescence resonance energy transfer between the dansyl fluorophore and protein tryptophan residues and could be used to (1) unambiguously assess active site binding of NS3 protease inhibitors, (2) directly det. equil. and pre-steady-state parameters of enzyme-inhibitor complex formation, and (3) dissect, using site-directed mutagenesis, the contribution of single residues of NS3 to inhibitor binding in direct binding assays. The assay was also used to characterize the inhibition of the NS3 protease by its cleavage products. We show that enzyme-product inhibitor complex formation depends on the presence of an NS4A cofactor peptide. Equil. and pre-steady-state data support an ordered mechanism of ternary (enzyme-inhibitor-cofactor) complex formation, requiring cofactor complexation prior to inhibitor binding.

IT 262437-54-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitor; probing the active site of the hepatitis C virus NS3 serine

proteinase by fluorescence resonance energy transfer)
 REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2000:68910 HCAPLUS
 DOCUMENT NUMBER: 132:245829
 TITLE: .alpha.-Ketoacids Are Potent Slow Binding Inhibitors
 of the Hepatitis C Virus NS3 Protease
 AUTHOR(S): Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania;
 Gerlach, Benjamin; Koch, Uwe; Biasiol, Gabriella;
 Fattori, Daniela; De Francesco, Raffaele; Matassa,
 Victor G.; Steinkuehler, Christian
 CORPORATE SOURCE: Departments of Biochemistry Medicinal Chemistry and
 Computational Chemistry, Istituto di Ricerche di
 Biologia Molecolare (IRBM) P. Angeletti, Pomezia,
 00040, Italy
 SOURCE: Biochemistry (2000), 39(7), 1849-1861
 CODEN: BICHAW; ISSN: 0006-2960
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The replication of the hepatitis C virus (HCV), an important human
 pathogen, crucially depends on the proteolytic maturation of a large viral
 polyprotein precursor. The viral nonstructural protein 3 (NS3) harbors a
 serine protease domain that plays a pivotal role in this process, being
 responsible for four out of the five cleavage events that occur in the
 nonstructural region of the HCV polyprotein. We here show that
 hexapeptide, tetrapeptide, and tripeptide .alpha.-ketoacids are potent,
 slow binding inhibitors of this enzyme. Their mechanism of inhibition
 involves the rapid formation of a noncovalent collision complex in a
 diffusion-limited, electrostatically driven assocn. reaction followed by a
 slow isomerization step resulting in a very tight complex. PH dependence
 expts. point to the protonated catalytic His 57 as an important
 determinant for formation of the collision complex. Ki values of the
 collision complexes vary between 3 nM and 18.5 .mu.M and largely depend on
 contacts made by the peptide moiety of the inhibitors. Site-directed
 mutagenesis indicates that Lys 136 selectively participates in
 stabilization of the tight complex but not of the collision complex. A
 significant solvent isotope effect on the isomerization rate const. is
 suggestive of a chem. step being rate limiting for tight complex
 formation. The potency of these compds. is dominated by their slow
 dissocn. rate consts., leading to complex half-lives of 11-48 h and
 overall Ki values between 10 pM and 67 nM. The rate consts. describing
 the formation and the dissocn. of the tight complex are relatively
 independent of the peptide moiety and appear to predominantly reflect the
 intrinsic chem. reactivity of the ketoacid function.

IT 252355-84-3P 262437-54-7P 262437-57-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(prepn. of .alpha.-ketoacids as potent slow binding inhibitors of
 hepatitis C virus NS3 protease)

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1999:795834 HCAPLUS
 DOCUMENT NUMBER: 132:36034
 TITLE: Preparation of peptide inhibitors of hepatitis C virus
 NS3 protease
 INVENTOR(S): Matassa, Victor; Narjes, Frank; Koehler, Konrad;

PATENT ASSIGNEE(S): Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
 Istituto Di Ricerche Di Biologia Molecolare P
 Angeletti S.p.A., Italy
 SOURCE: PCT Int. Appl., 121 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964442	A1	19991216	WO 1999-GB1824	19990609
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RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2330247	AA	19991216	CA 1999-2330247	19990609
AU 9942798	A1	19991230	AU 1999-42798	19990609
AU 754773	B2	20021121		
EP 1084137	A1	20010321	EP 1999-955475	19990609
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE			
PRIORITY APPLN. INFO.:			GB 1998-12523	A 19980610
			WO 1999-GB1824	W 19990609

AB Fluorinated oligopeptides Y-B-A-X or Y-B-A'-X' [A is an amino acid residue NHCH(CH₂CHF₂)(CH₂)_mCO and A' is NHCHR₁(CH₂)_mCO (m = 0, 1; R₁ is a fluorine-substituted hydrocarbyl side chain); B is a naturally or non-naturally occurring amino acid residue NHCHR₂CO (R₂ is a nonpolar or polar but uncharged side chain or is a side chain contg. an acidic functionality); X = CO₂R₈, H, OR₈, CF₃, CONR₉R₁₀, NHSO₂R₂₅, or certain 5-membered heterocyclic groups (R₈, R₉, R₁₀, R₂₅ = H, alkyl, alkenyl, aryl, aralkyl); X' = NHSO₂N₂₅; Y = Z-F-E-D-C (C is a natural or non-natural amino acid residue having non-polar, polar but uncharged, or acidic side chains; D, E, and F may be absent or represent a natural or non-natural amino acid; Z is absent, H, or R₇CO which forms an amide, urethane, or urea linkage with the nitrogen atom to which it is attached) or R₁₃CO (R₁₃ is an aliph. or arom. group contg. 1-25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms, and up to 9 other heteroatoms)] were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, Ac-Asp-Glu-Met-Glu-Glu-NHCH(CH₂CHF₂)CO₂H-(S), prepd. by coupling of (S)-tert-Bu 2-amino-4,4-difluorobutanoate hydrochloride with protected pentapeptide, showed IC₅₀ for inhibition of NS3 protease.

IT 252355-84-3P 252355-85-4P 252355-86-5P
 252355-87-6P 252355-88-7P 252355-89-8P
 252355-90-1P 252355-91-2P 252355-93-4P
 252355-94-5P 252355-95-6P 252355-96-7P
 252355-97-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> fil caold

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> fil reg

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STRUCTURE FILE UPDATES: 28 SEP 2003 HIGHEST RN 594810-89-6
DICTIONARY FILE UPDATES: 28 SEP 2003 HIGHEST RN 594810-89-6

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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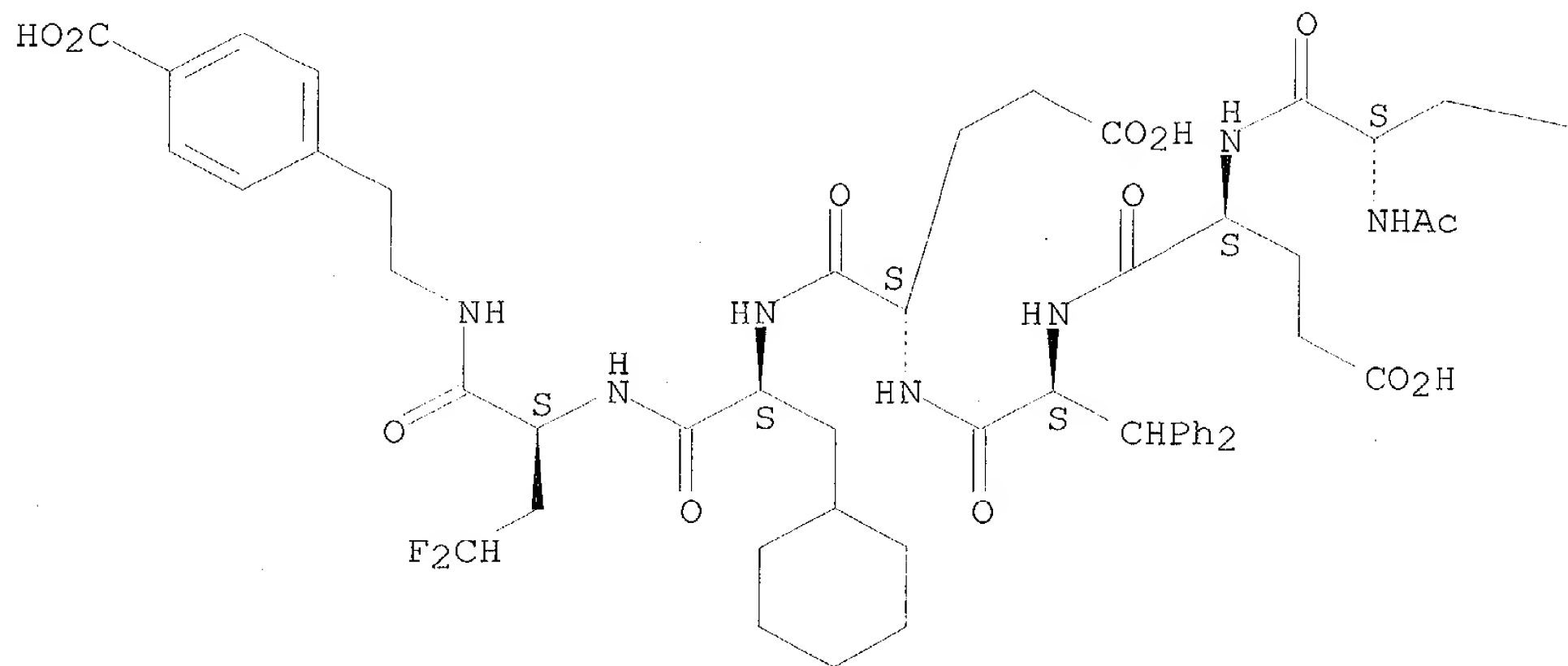
L5 ANSWER 1 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 467440-45-5 REGISTRY
CN Butanamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-N-[2-(4-carboxyphenyl)ethyl]-4,4-difluoro-, (2S)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH

MF C53 H65 F2 N7 O15
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

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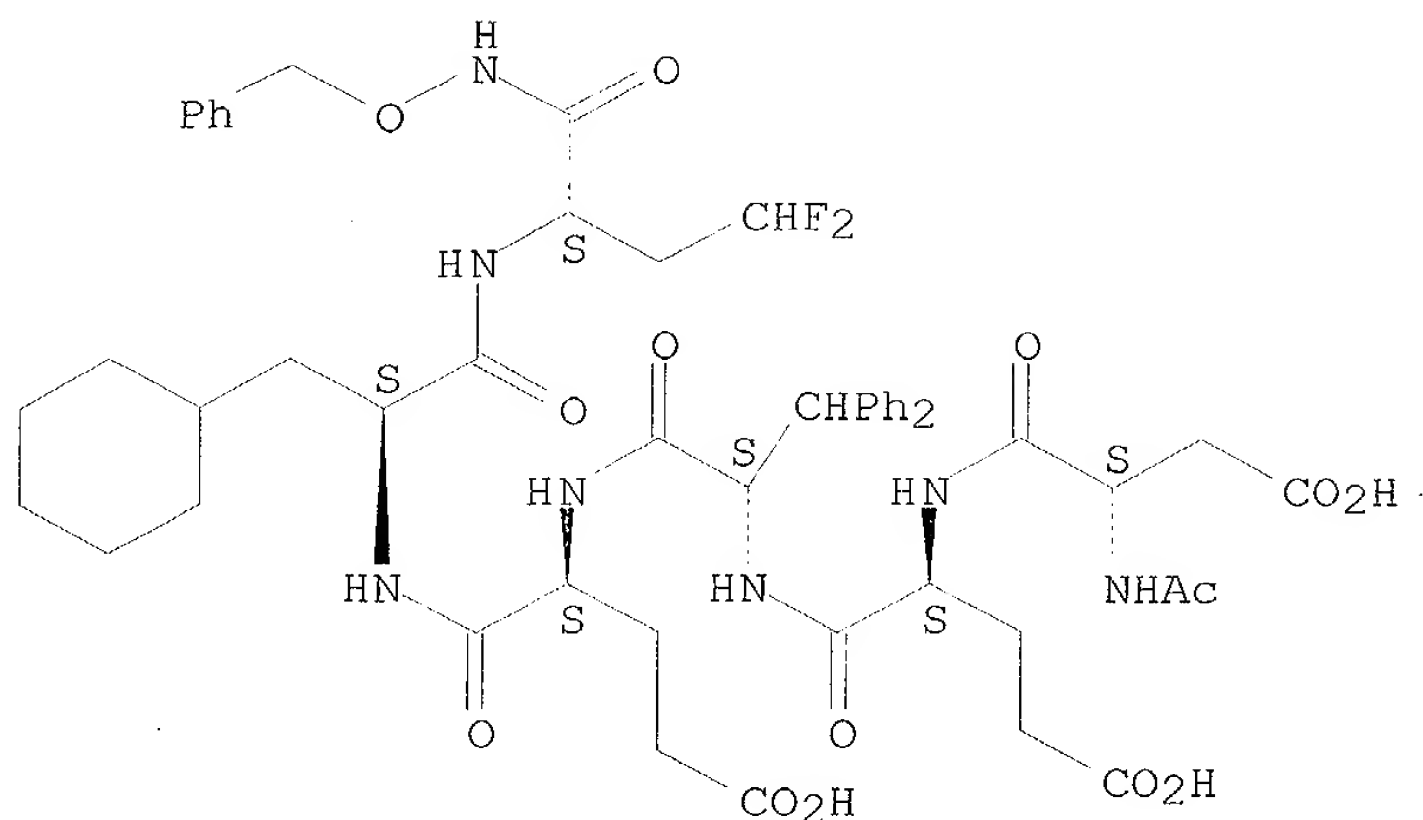
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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:295254

L5 ANSWER 2 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 467440-28-4 REGISTRY
 CN Butanamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-difluoro-N-(phenylmethoxy)-, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C51 H63 F2 N7 O14
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



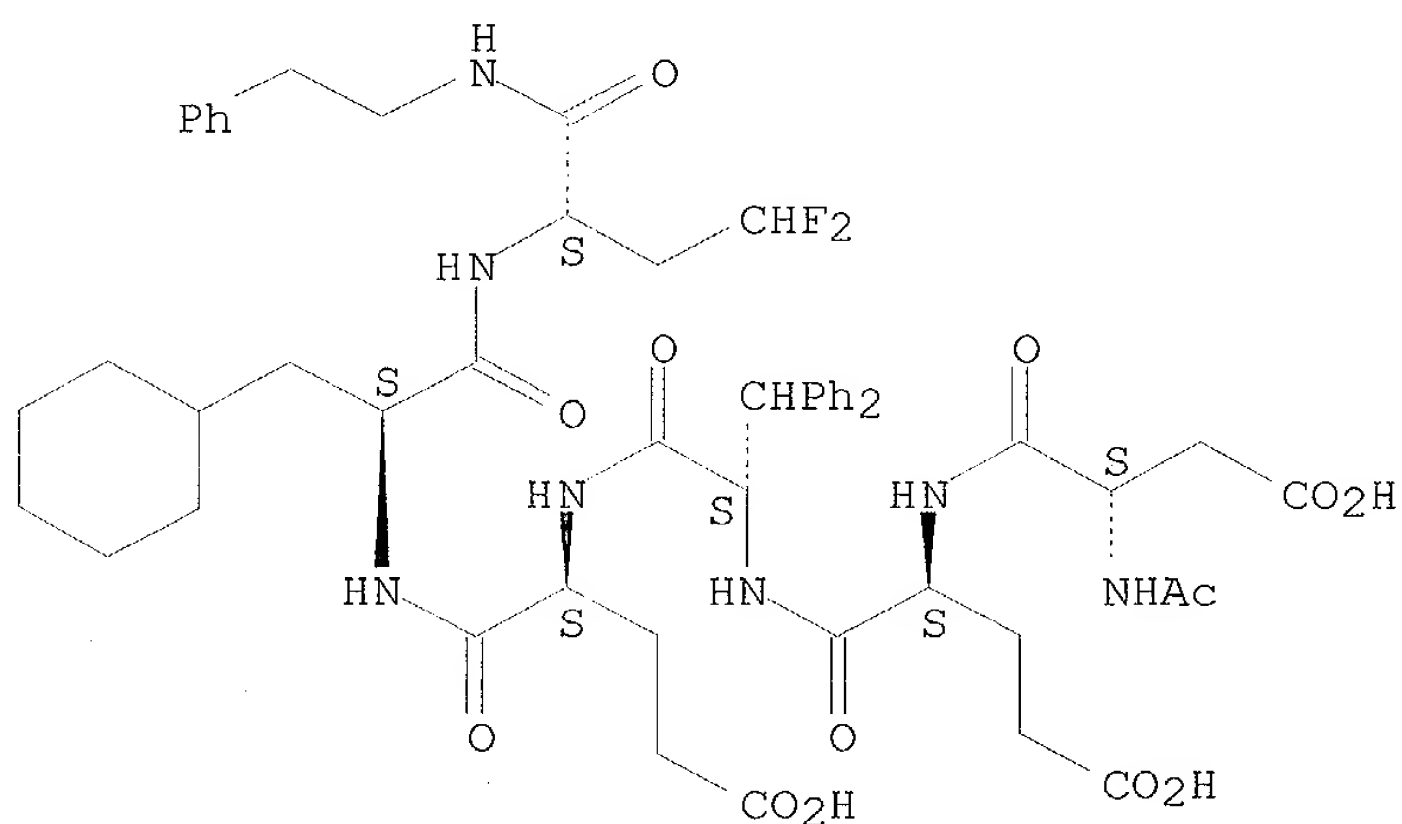
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:295254

L5 ANSWER 3 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 467440-27-3 REGISTRY
CN Butanamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-difluoro-N-(2-phenylethyl)-, (2S)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C52 H65 F2 N7 O13
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



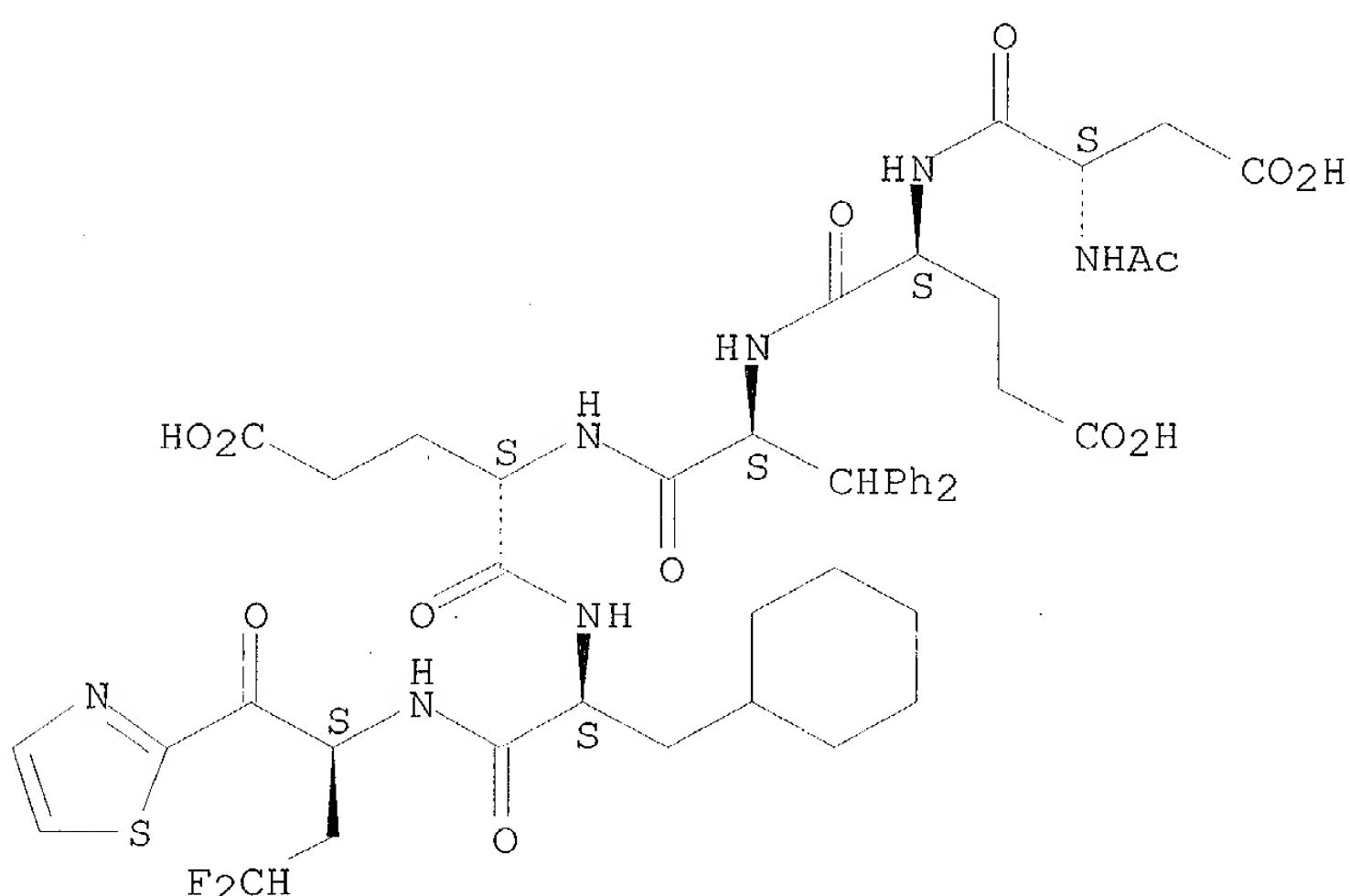
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:295254

L5 ANSWER 4 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 444990-70-9 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-3,3-difluoro-1-(2-thiazolylcarbonyl)propyl]- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C47 H57 F2 N7 O13 S
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



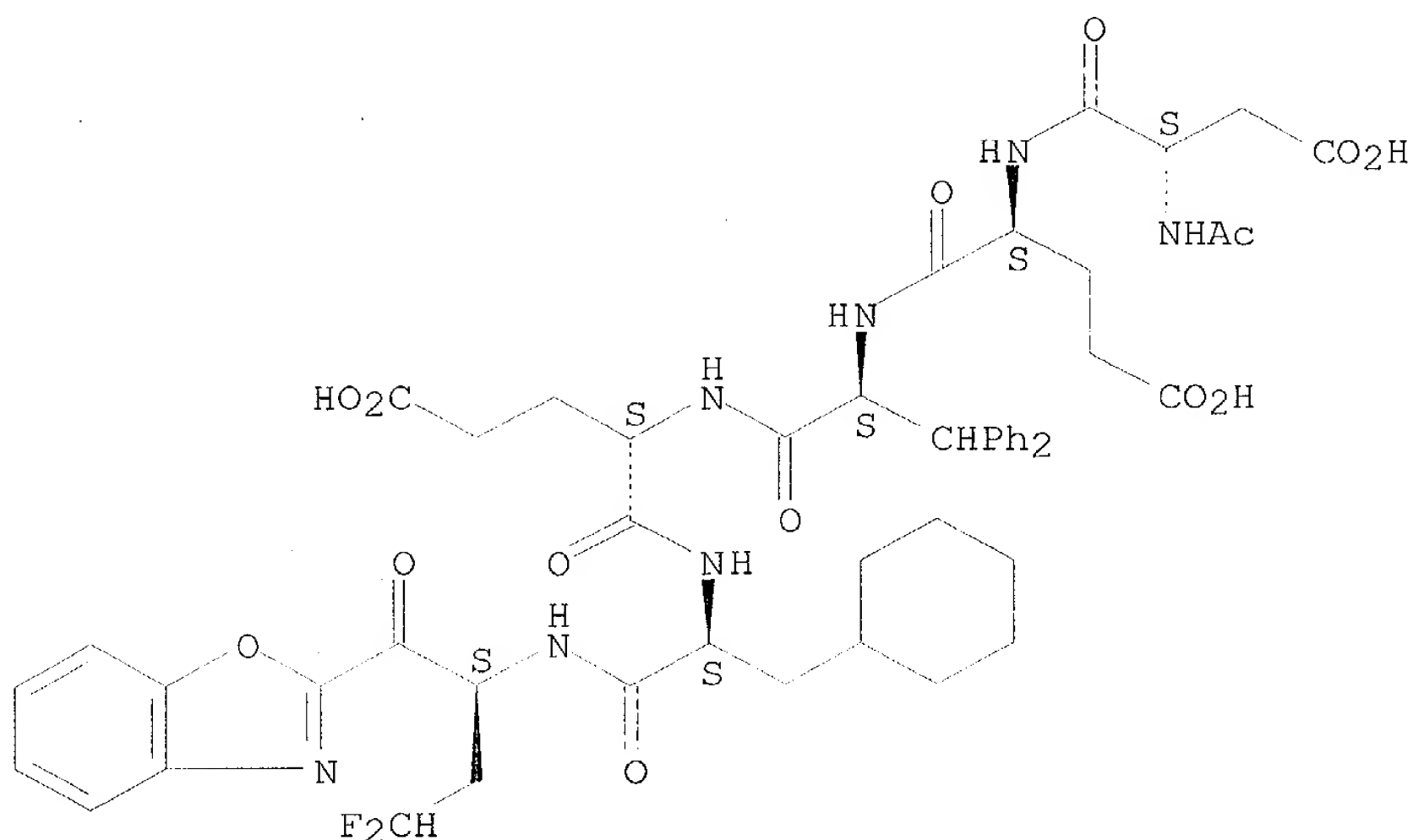
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 5 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 444990-69-6 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1S)-1-(2-benzoxazolylcarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C51 H59 F2 N7 O14
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



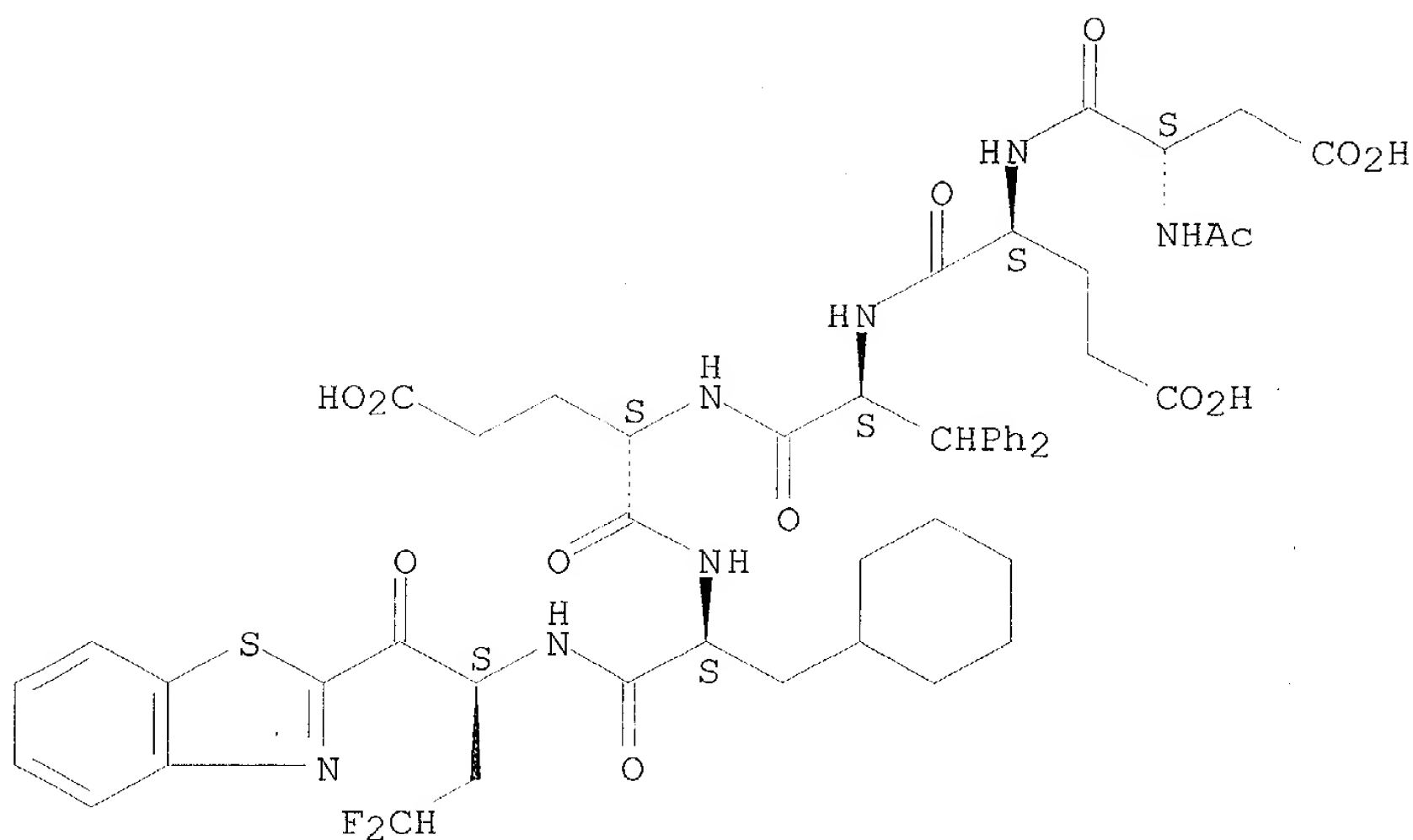
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 6 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 444990-68-5 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1S)-1-(2-
benzothiazolylcarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX
NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C51 H59 F2 N7 O13 S
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



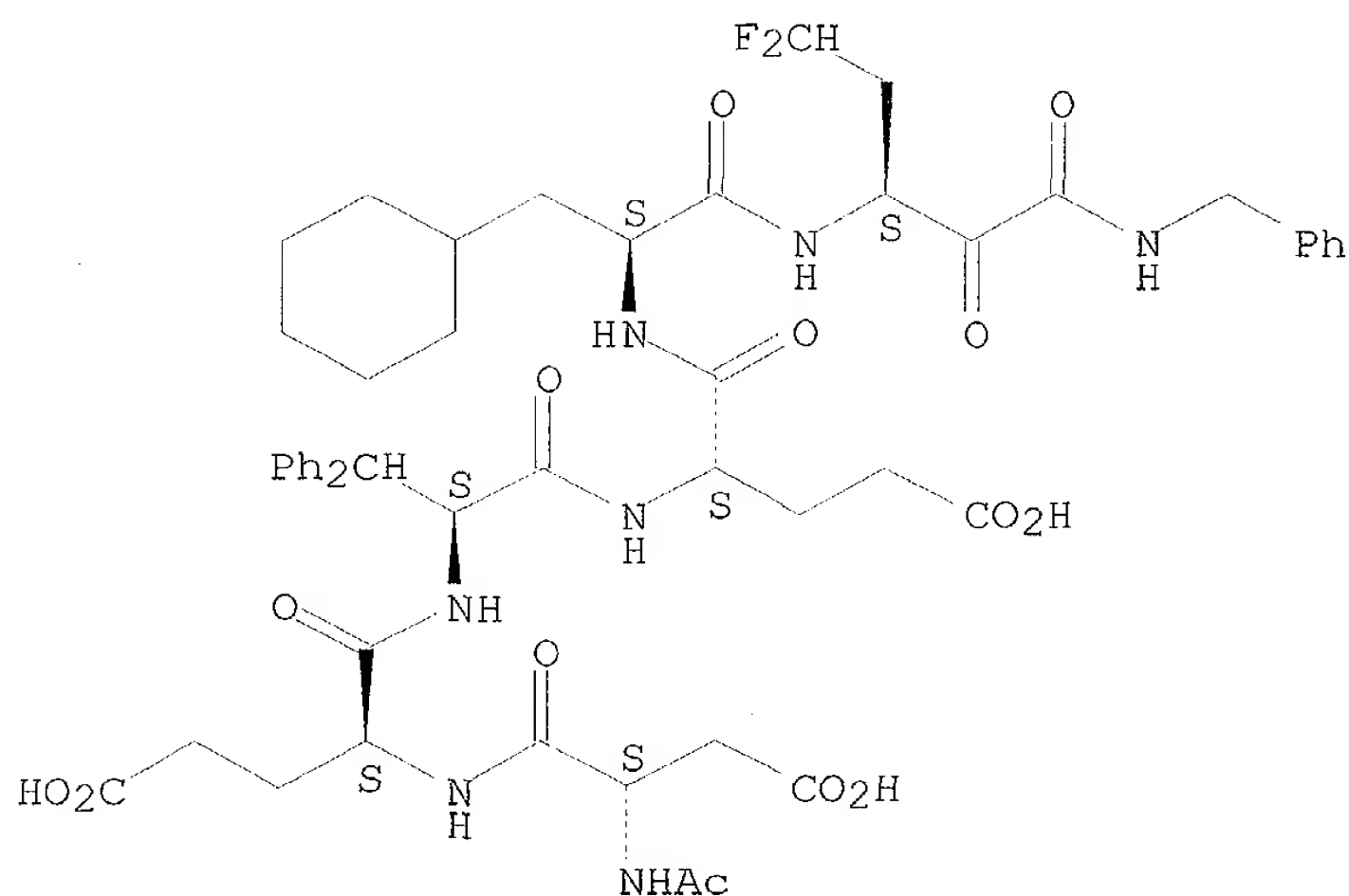
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 7 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 444990-67-4 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-1-(2,2-difluoroethyl)-2,3-dioxo-3-[(phenylmethyl)aminolpropyl]- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C52 H63 F2 N7 O14
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



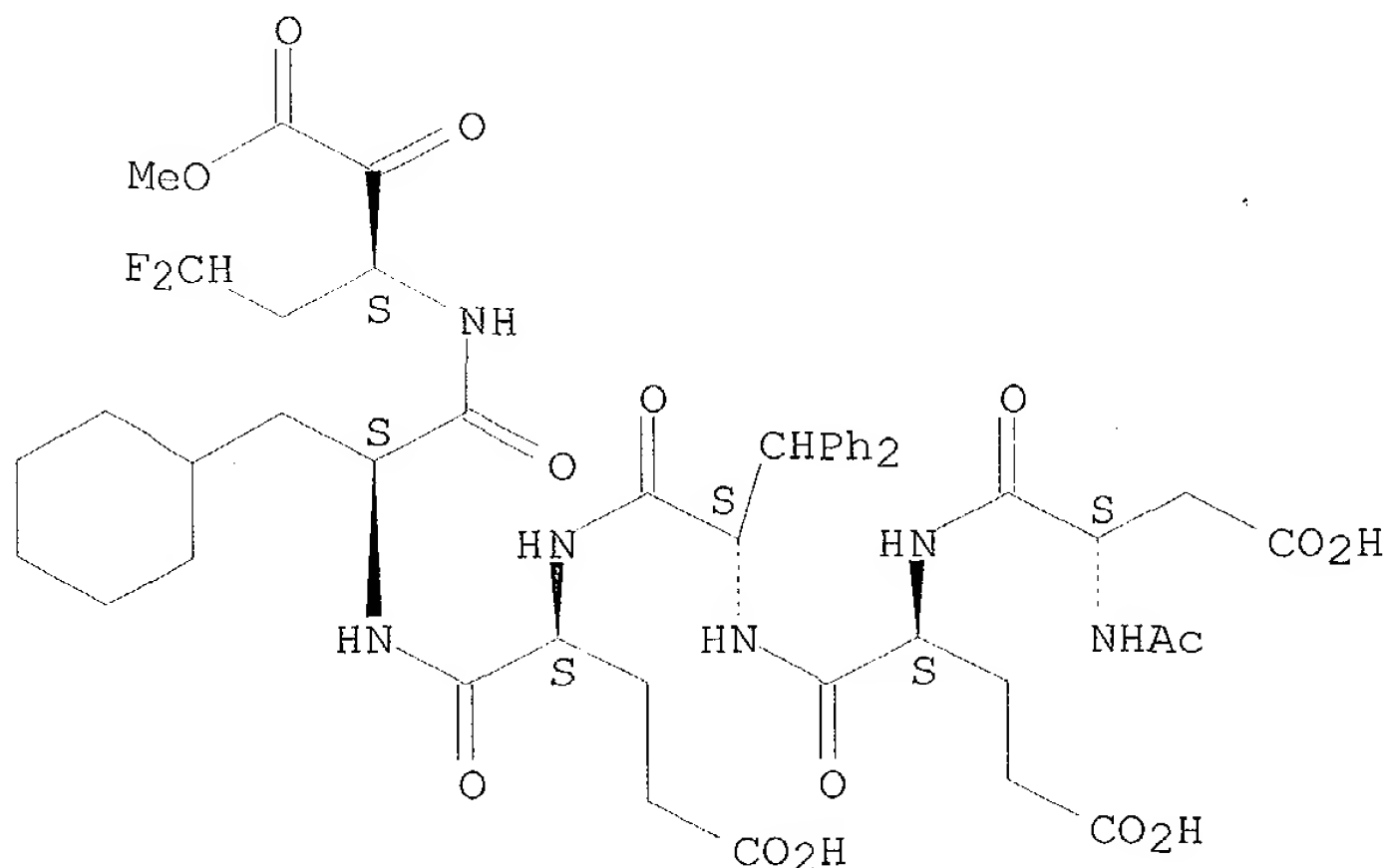
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 8 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 444990-66-3 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-1-(2,2-difluoroethyl)-3-methoxy-2,3-dioxopropyl]- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C46 H58 F2 N6 O15
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

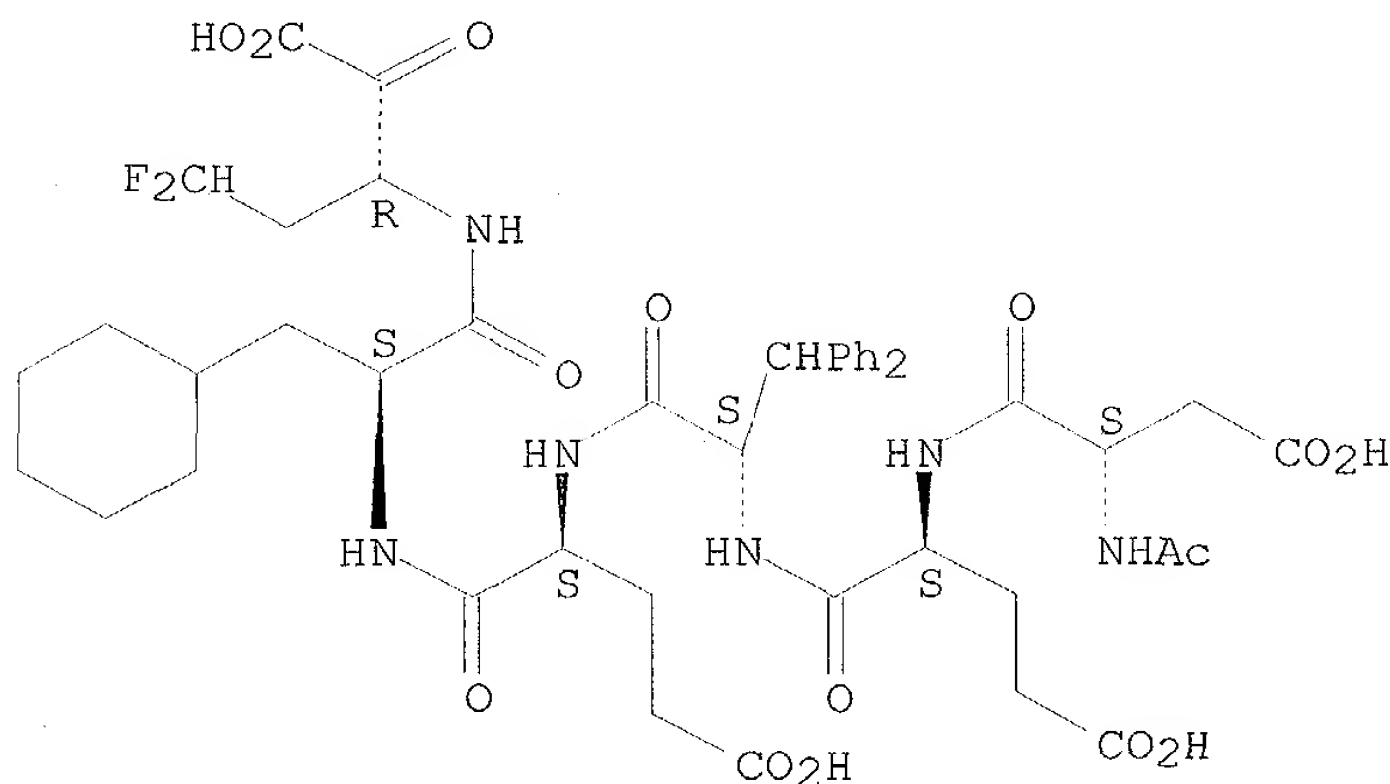
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 9 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 262437-57-0 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1R)-1-(carboxycarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C45 H56 F2 N6 O15
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



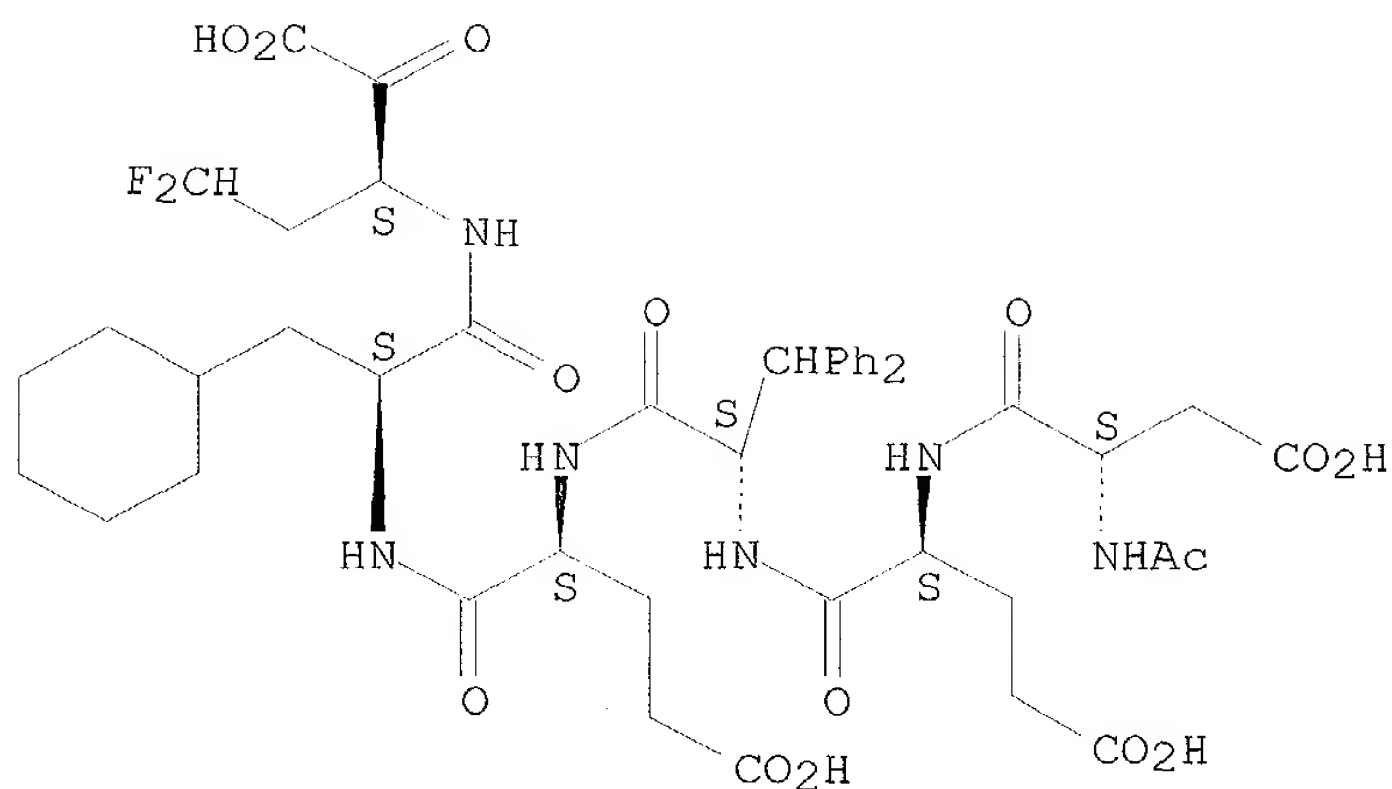
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:245829

L5 ANSWER 10 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 262437-54-7 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1S)-1-(carboxycarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C45 H56 F2 N6 O15
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



4 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

REFERENCE 2: 137:47425

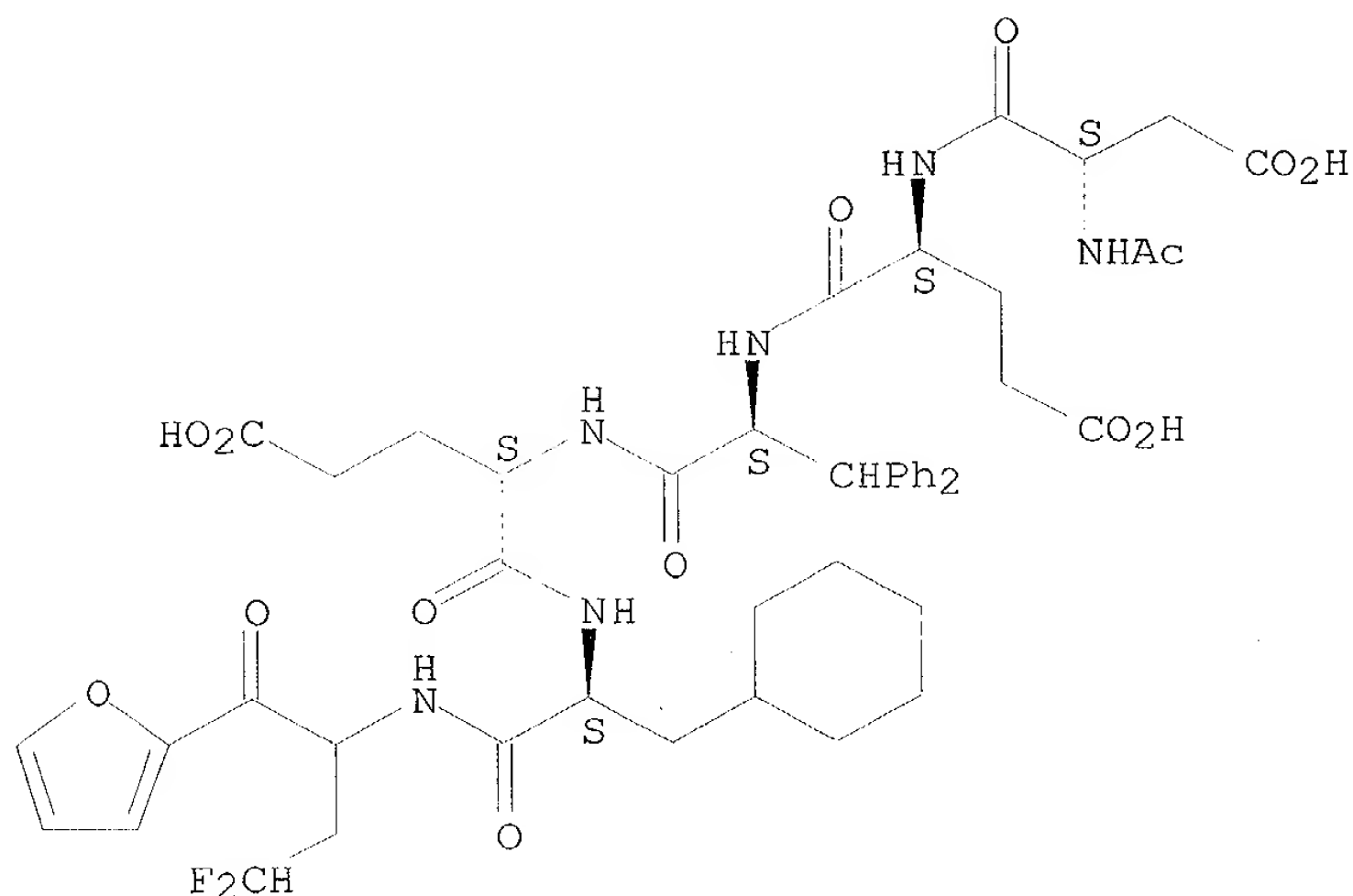
REFERENCE 3: 133:189820

REFERENCE 4: 132:245829

L5 ANSWER 11 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 252355-97-8 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[3,3-difluoro-1-(2-
 furanylcarbonyl)propyl]- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C48 H58 F2 N6 O14
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



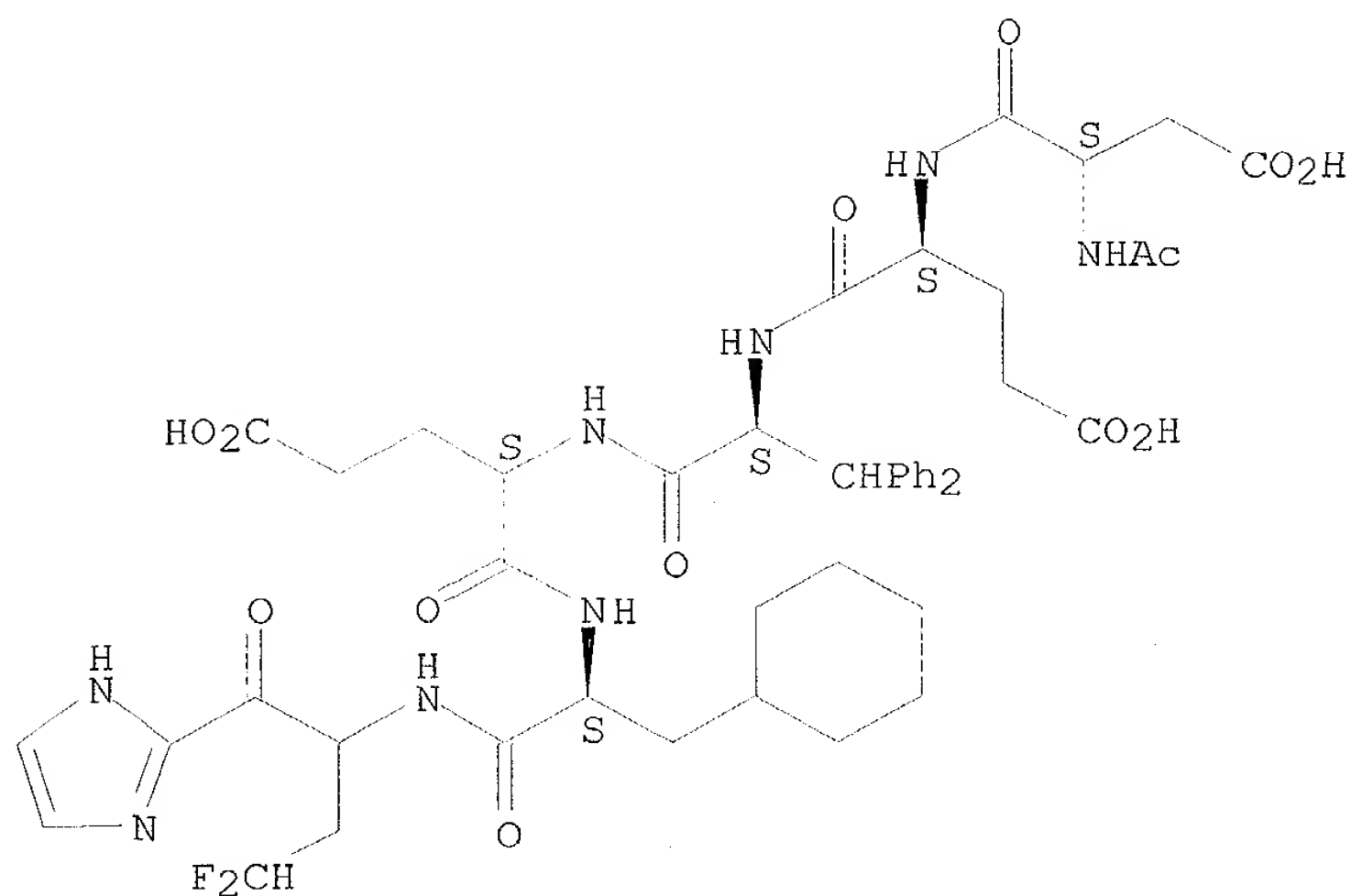
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 12 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-96-7 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[3,3-difluoro-1-
(1H-imidazol-2-ylcarbonyl)propyl]- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C47 H58 F2 N8 O13
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



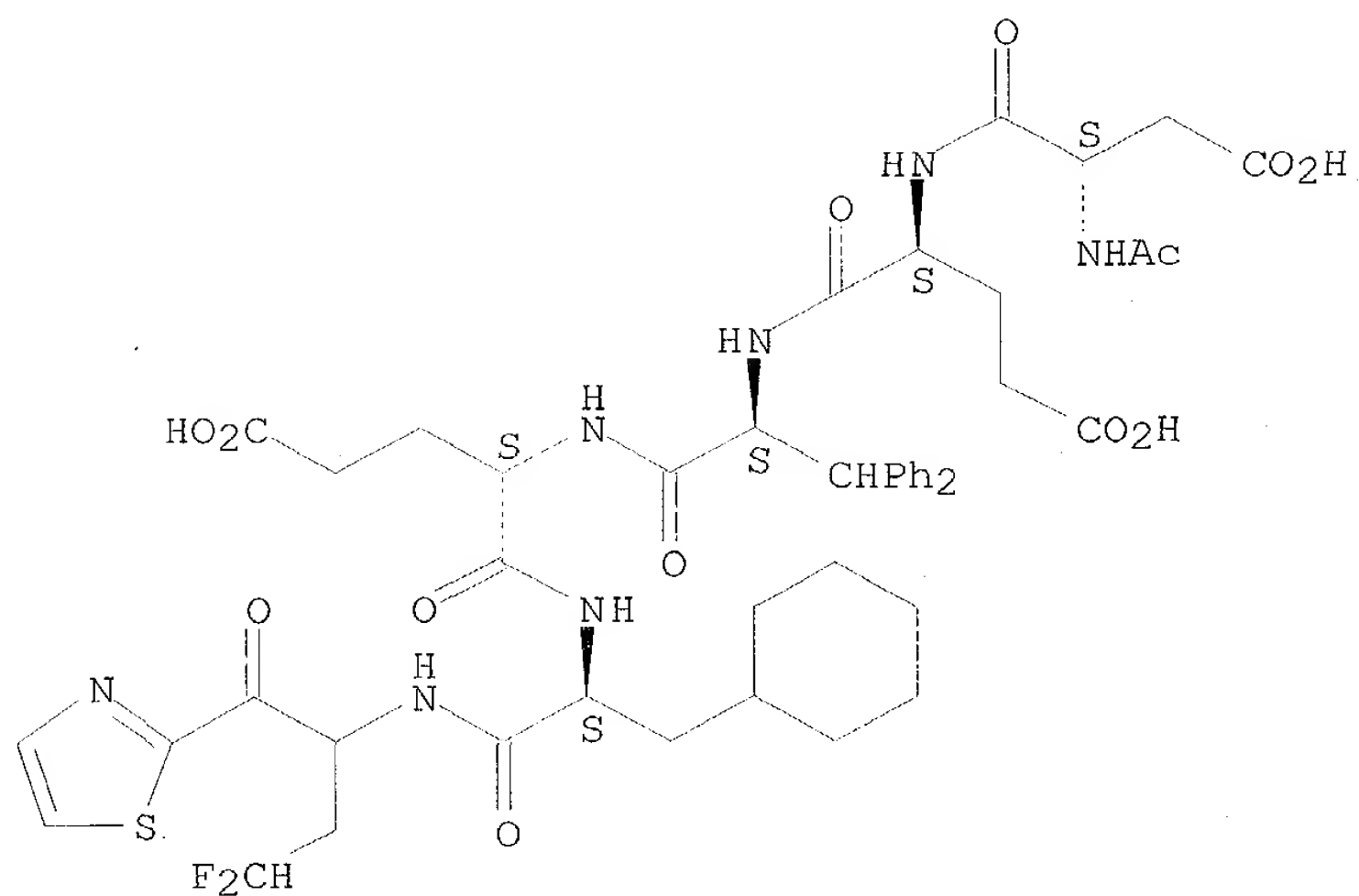
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 13 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-95-6 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[3,3-difluoro-1-(2-thiazolylcarbonyl)propyl]- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C47 H57 F2 N7 O13 S
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



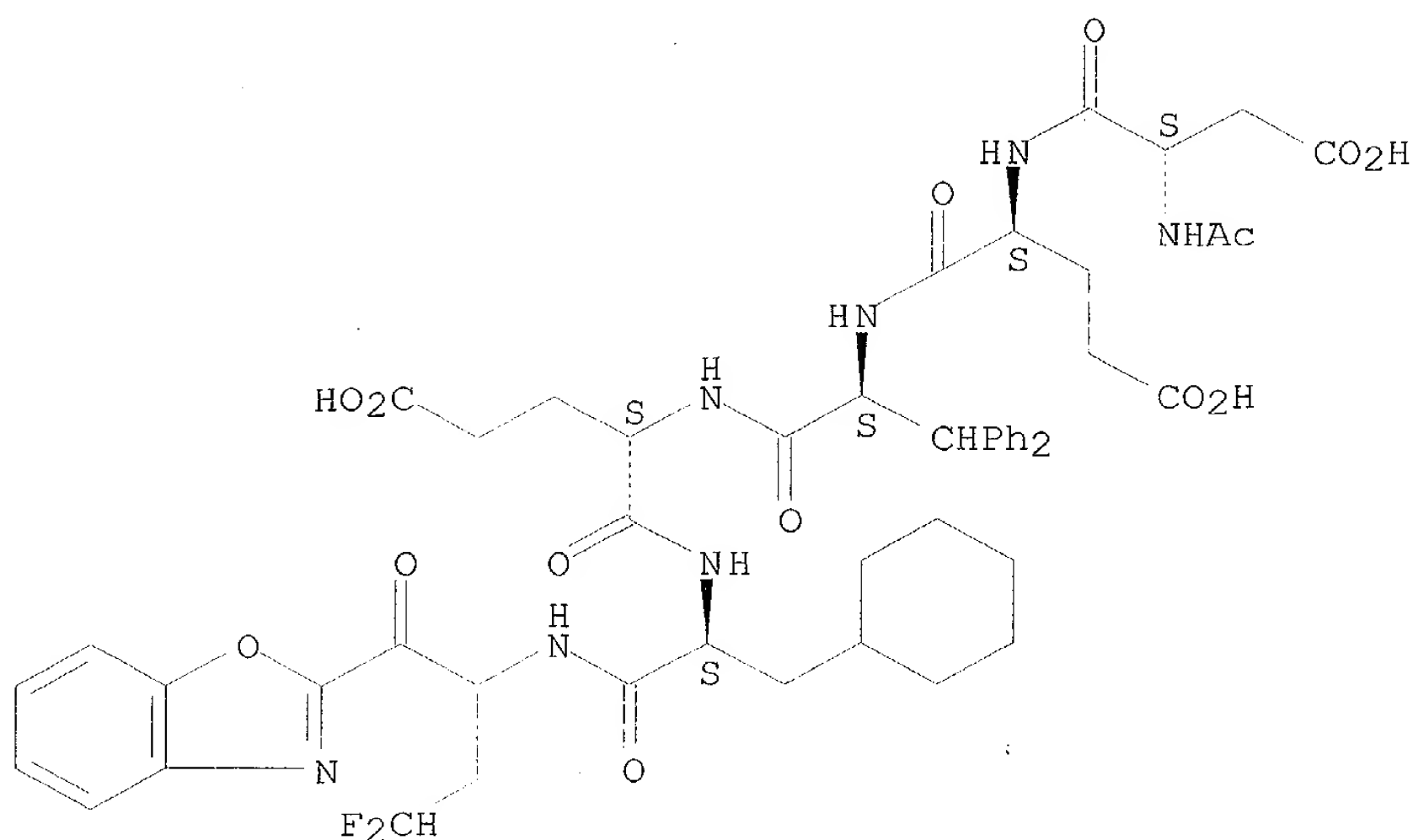
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 14 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-94-5 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[1-(2-benzoxazolylcarbonyl)-3,3-
difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C51 H59 F2 N7 O14
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



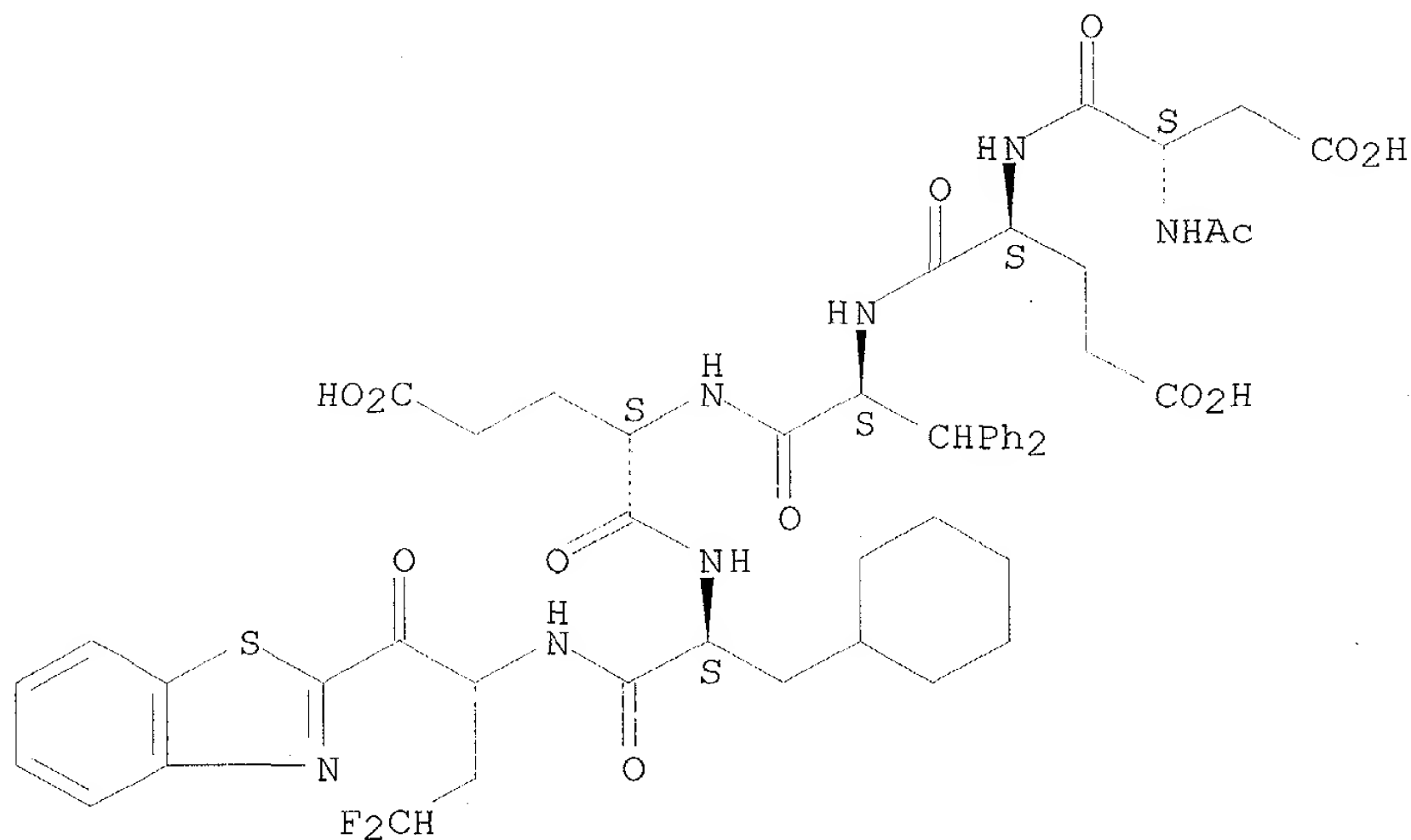
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 15 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-93-4 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[1-(2-benzothiazolylcarbonyl)-
3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C51 H59 F2 N7 O13 S
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



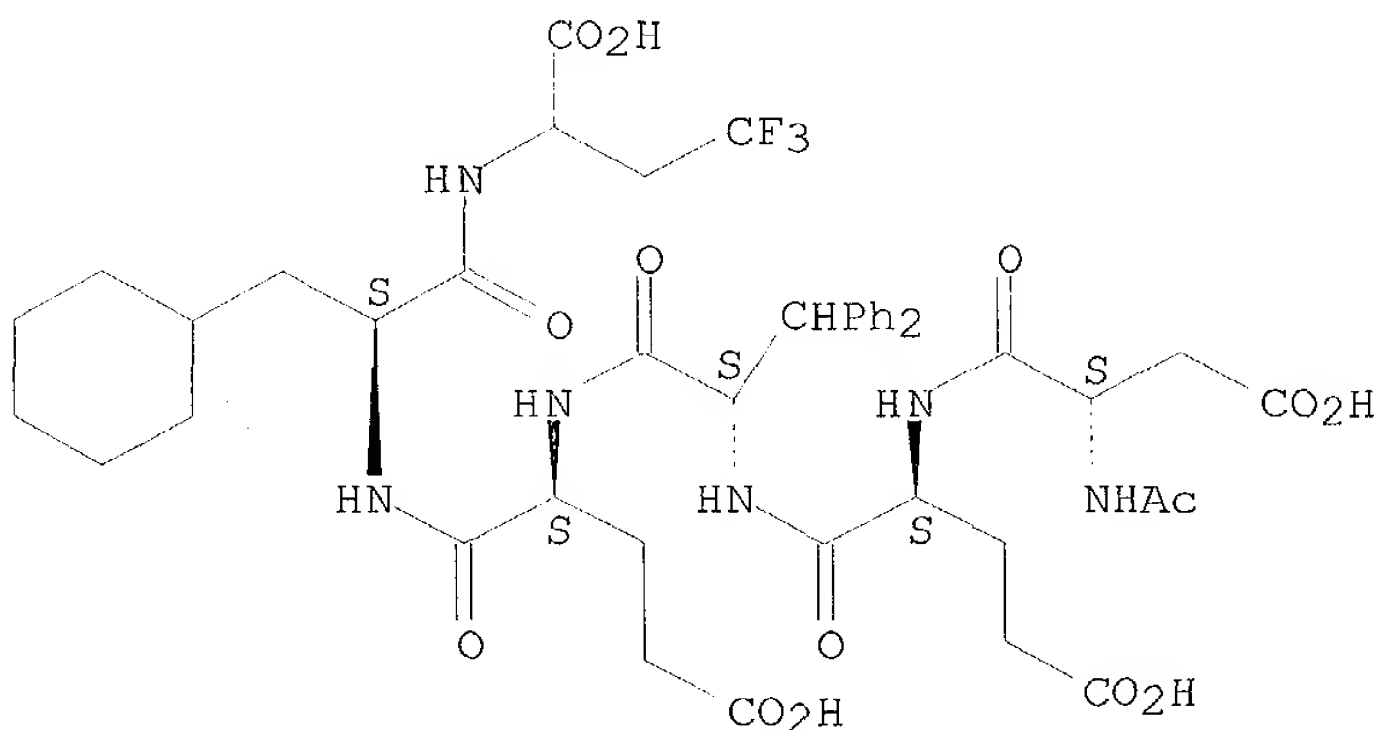
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 16 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-91-2 REGISTRY
CN Butanoic acid, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4,4-trifluoro- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C44 H55 F3 N6 O14
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



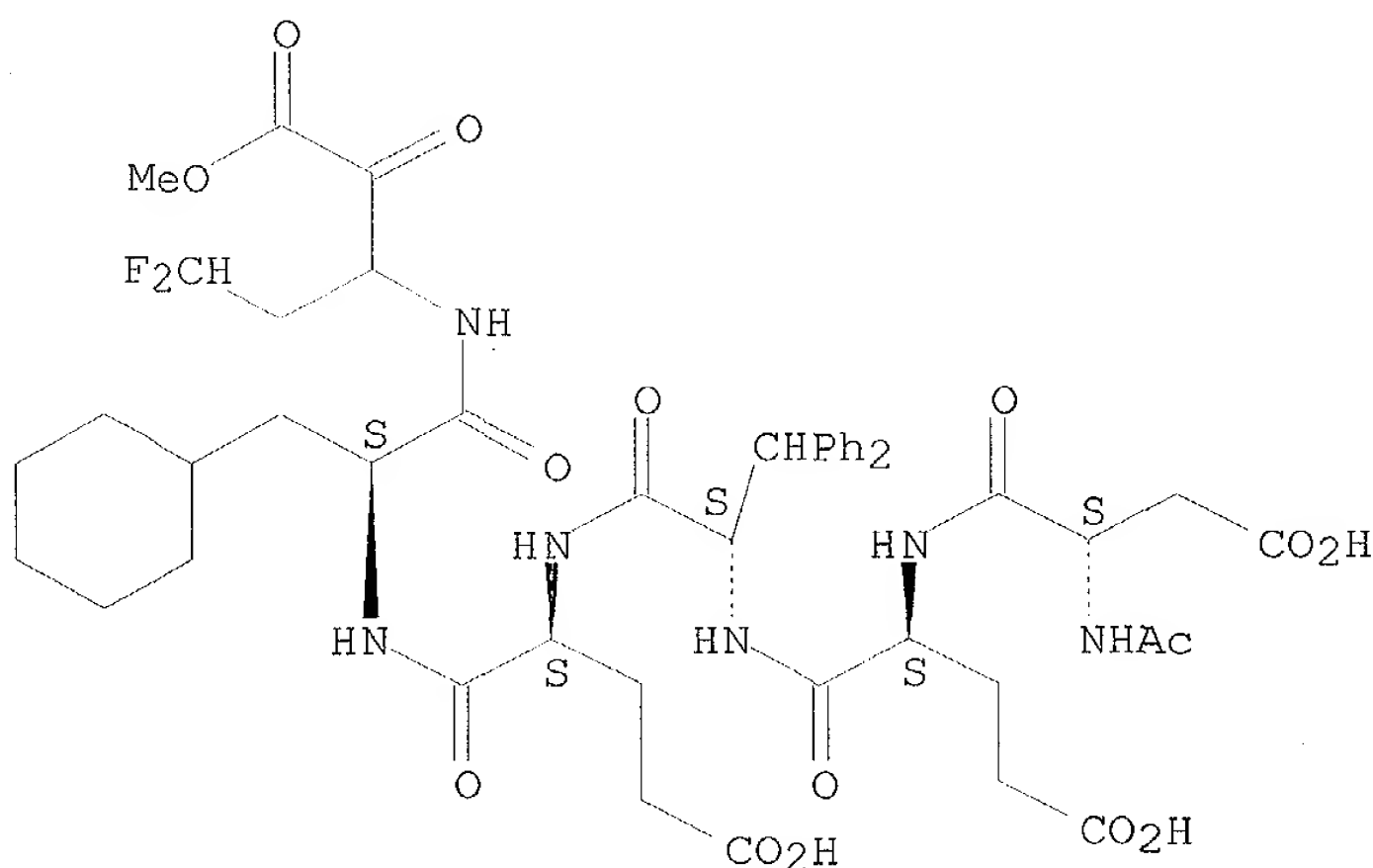
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 17 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 252355-90-1 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[1-(2,2-difluoroethyl)-3-methoxy-2,3-dioxopropyl]- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C46 H58 F2 N6 O15
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



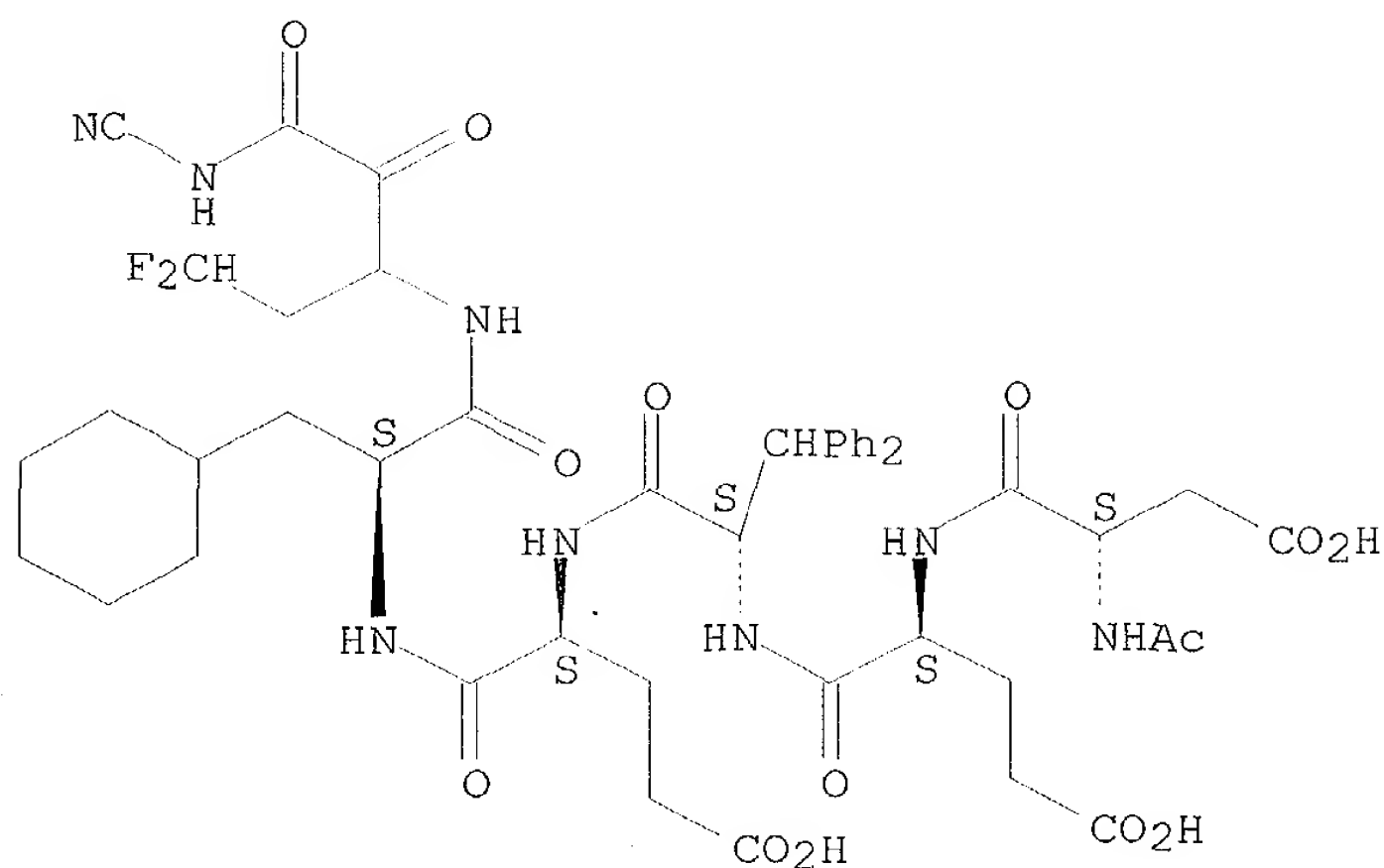
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 18 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 252355-89-8 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[3-(cyanoamino)-1-(2,2-difluoroethyl)-2,3-dioxopropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C46 H56 F2 N8 O14
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



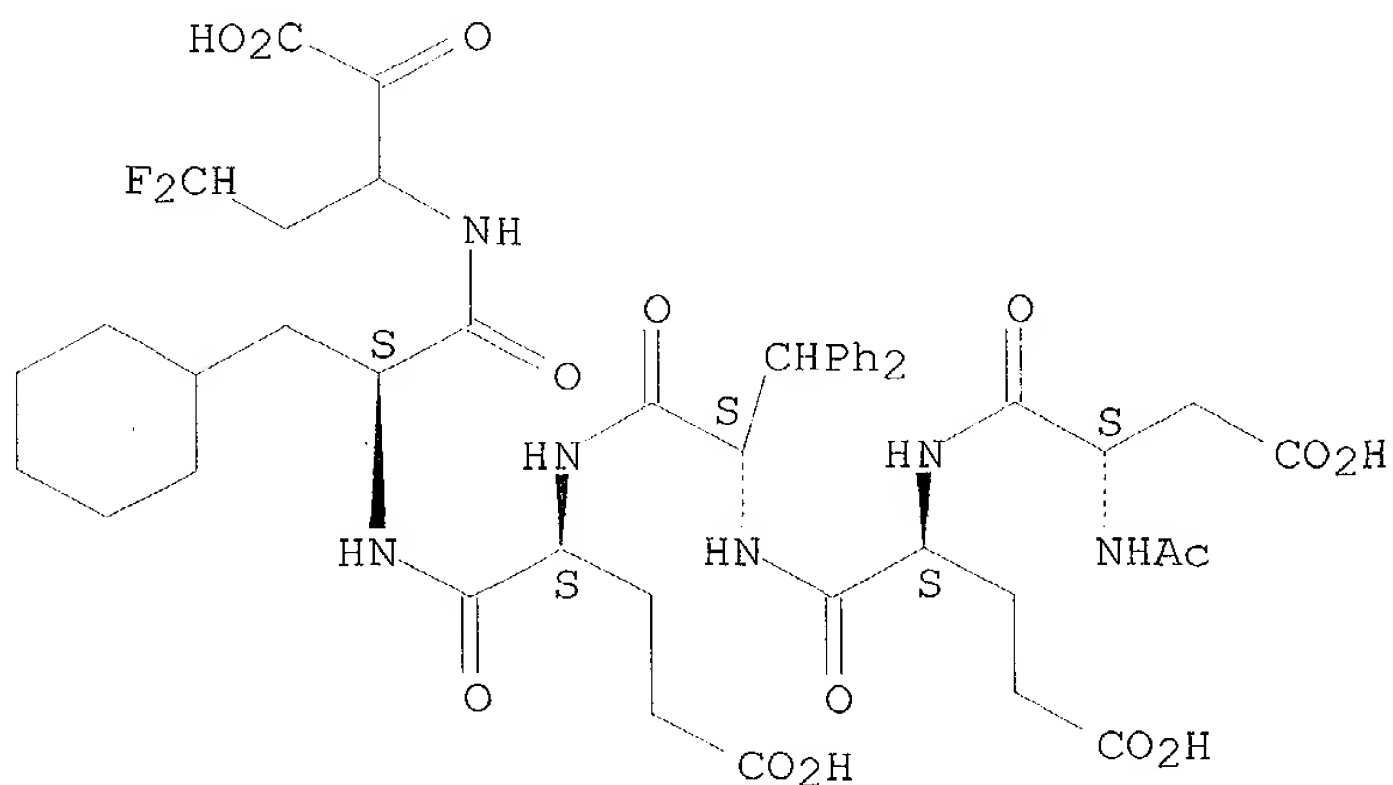
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 19 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-88-7 REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[1-(carboxycarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C45 H56 F2 N6 O15
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



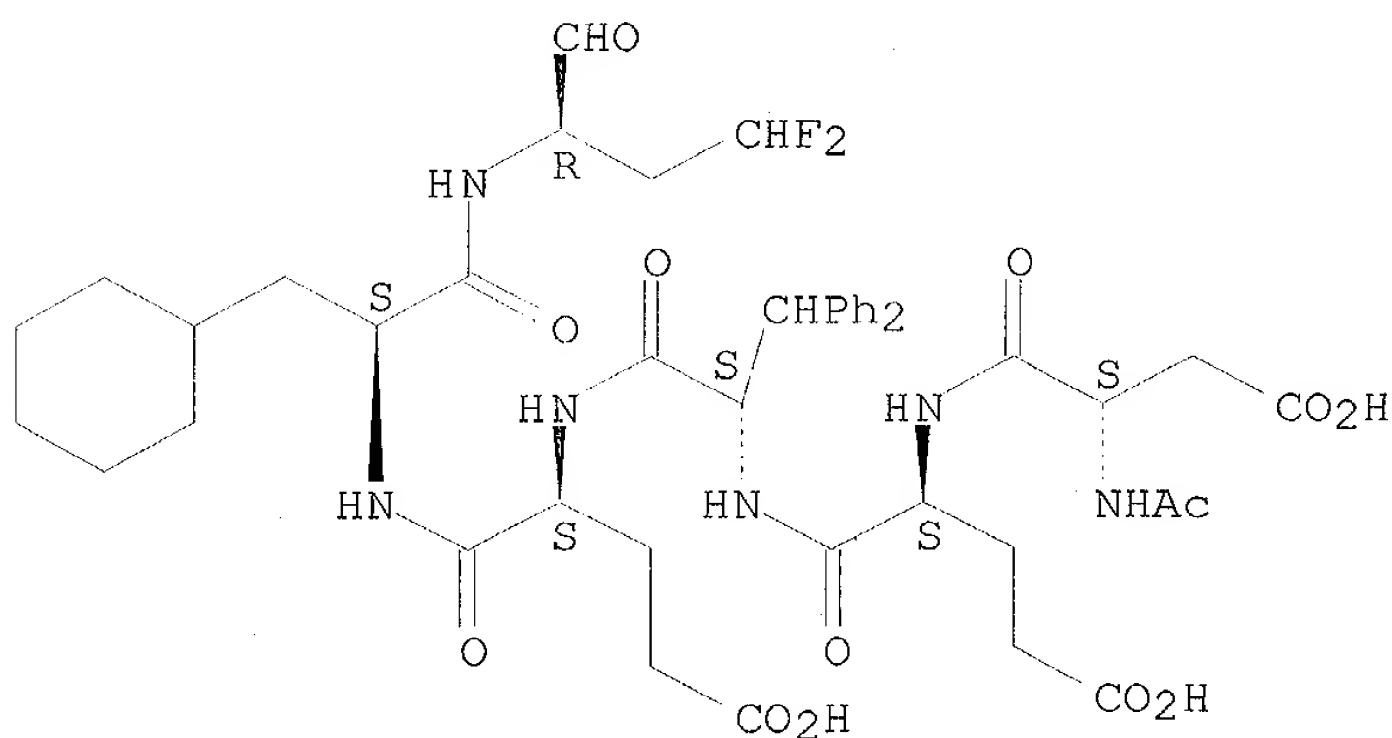
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 20 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 252355-87-6 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1R)-3,3-difluoro-1-formylpropyl]- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C44 H56 F2 N6 O13
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



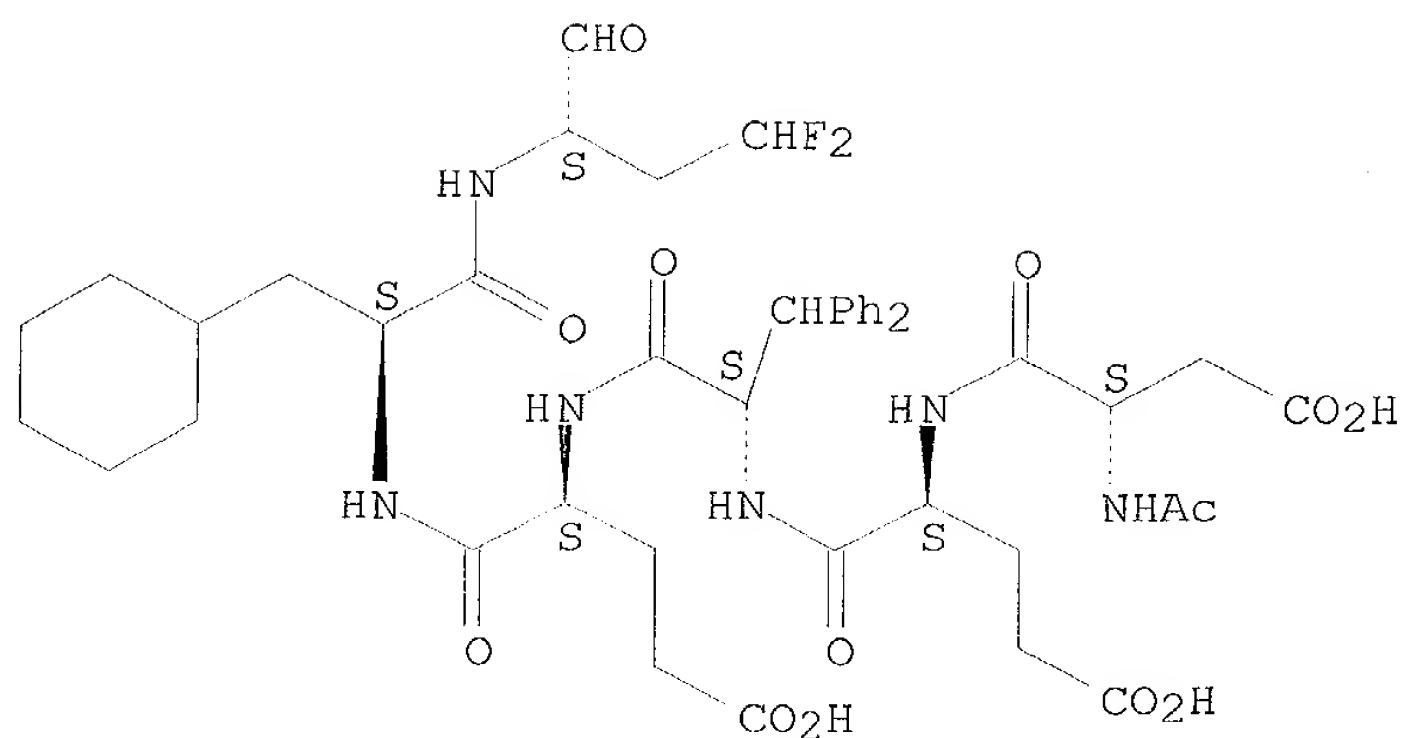
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 21 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 252355-86-5 REGISTRY
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-3,3-difluoro-1-formylpropyl]- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C44 H56 F2 N6 O13
 SR CA
 LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

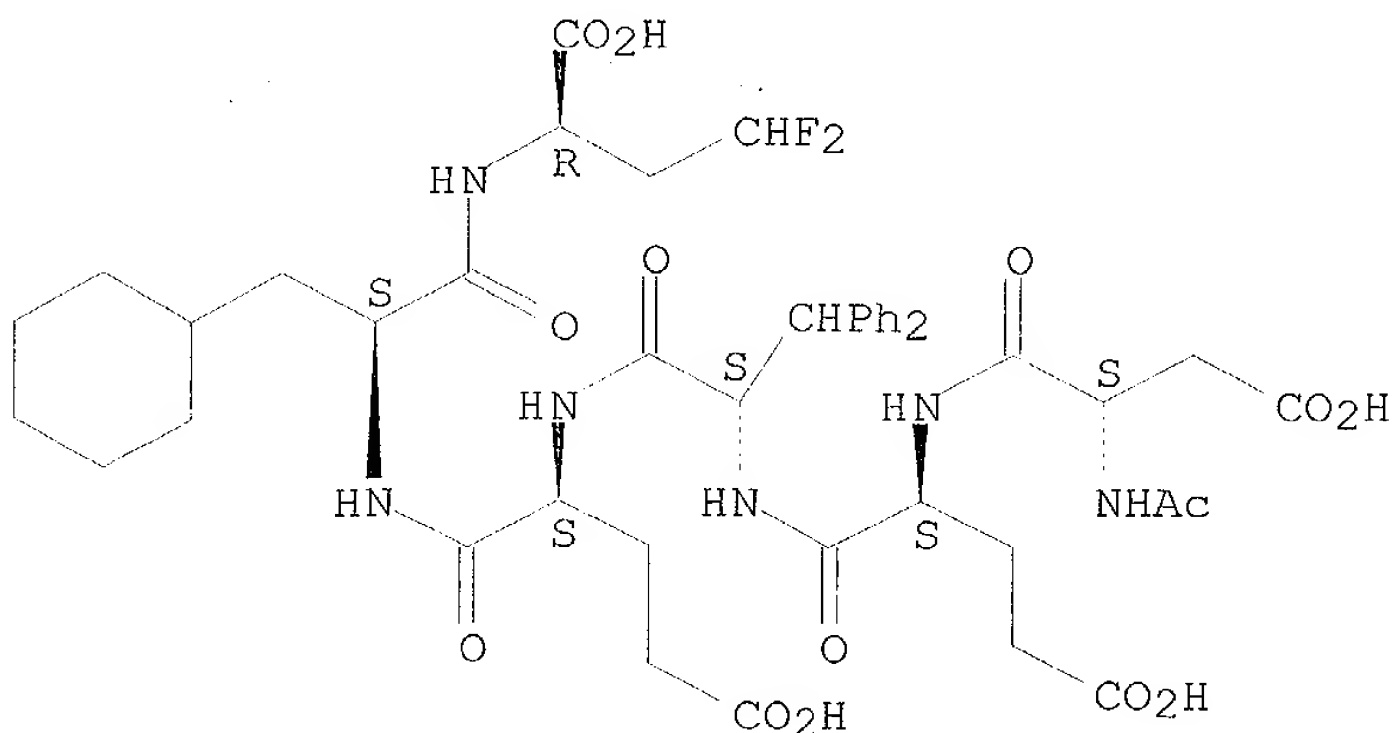
REFERENCE 1: 137:149812

REFERENCE 2: 132:36034

L5 ANSWER 22 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
RN 252355-85-4 REGISTRY
CN Butanoic acid, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-difluoro-, (2R)- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C44 H56 F2 N6 O14
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

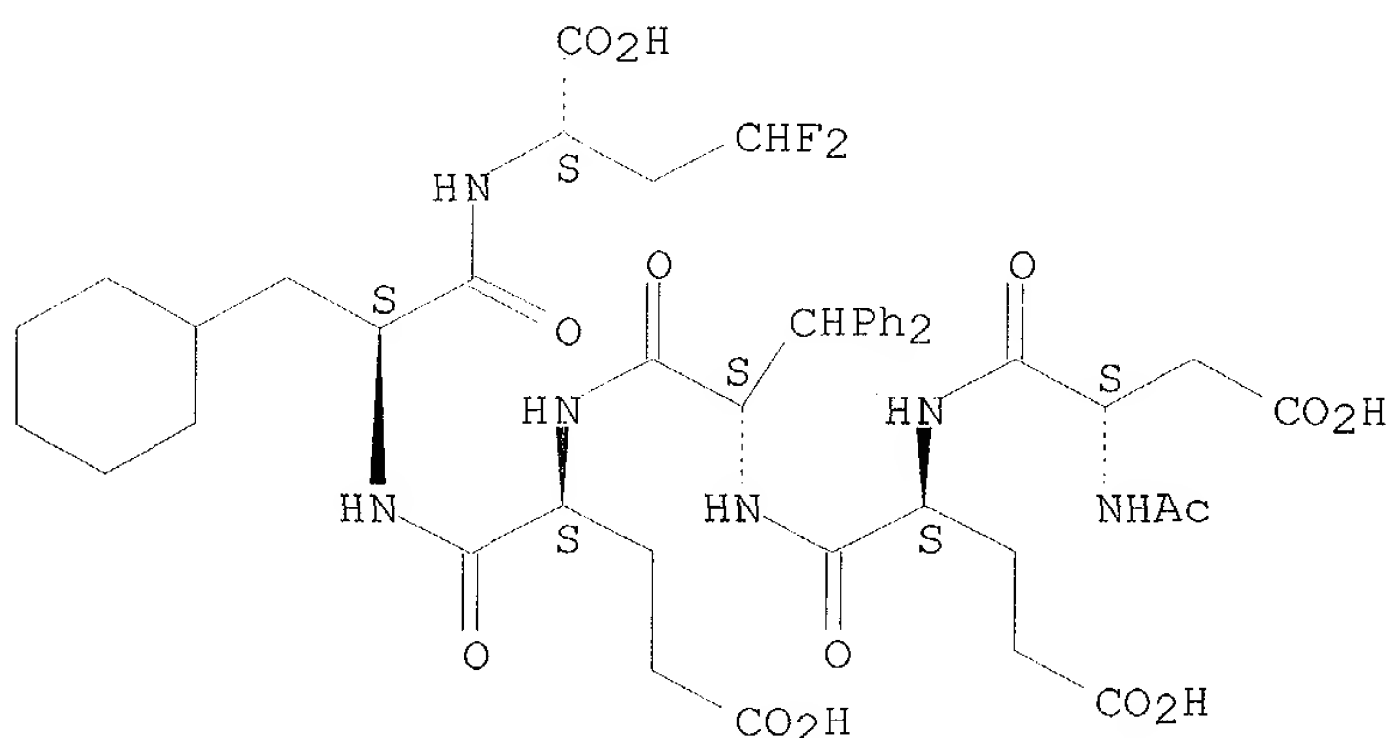
REFERENCE 1: 137:149812

REFERENCE 2: 132:36034

L5 ANSWER 23 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 252355-84-3 REGISTRY
 CN Butanoic acid, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-
 difluoro-, (2S)- (9CI) (CA INDEX NAME)
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF C44 H56 F2 N6 O14
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812
 REFERENCE 2: 132:245829
 REFERENCE 3: 132:36034